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Study of positron surface states on the alkali-metal-covered transition-metal surface

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Abstract

We present a first-principles study of annihilation probabilities of surface trapped positrons with core electrons at the Cu(100) surface with sub-monolayers of Cs adsorbed. Image-potential-induced positron surface states are calculated using a corrugated-mirror model in a full three-dimensional geometry. These states are studied for various arrangements of Cs atoms below and above the critical alkali-metal coverage of approximately 0.7 physical monolayer. Computer simulations of the deposition of Cs atoms are used to show that hexagonal close-packed Cs islands are formed at about 0.7 physical monolayer coverage of Cs. It is found that the abrupt decrease in the positron annihilation rate with Cu 3p electrons observed experimentally results from a metallization of the Cs islands. This causes a shift in the localization of the positron bound state from the Cs/Cu interface to the vacuum side of the Cs overlayer, with the corresponding abrupt decrease in the positron annihilation probability with Cu electrons. Annihilation probabilities for positrons with Cs electrons are also computed and compared with experiment.

1. Introduction

Alkali-metal adsorption on transition-metal surfaces has been studied with increasing interest due to the wide variety of electronic properties which are important from both fundamental and technological points of view [1–10]. Recently alkali-metal adsorption on transition-metal surfaces has become the subject of experimental studies using a new surface characterization technique, the positron-annihilation-induced Auger electron spectroscopy (PAES) [11–16]. It has been found in PAES studies of the Cs/Cu(100) system that the normalized intensity of the positron-annihilation-induced Cu $M_{2,3}VV$ Auger signal drops sharply almost to zero at 163 K in a range of less than 0.02 monolayer wide at the critical Cs coverage of 0.7 physical monolayer. Thus the positron annihilation rate with the Cu 3p electrons has demonstrated a sharp transition from high annihilation rates to very low annihilation rates when the Cs coverage reaches 0.7 physical monolayer. These PAES results significantly deviate from predictions of the Nieminen–Jensen (NJ) theory [11,17], according to which the positron becomes localized in the region between the substrate and the alkali-metal overlayer up to the coverage of one physical monolayer. This location of the positron predicts the insensitivity of the positron annihilation probability with Cu electrons to changes in the Cs adsorbate density. Thus, according to the NJ theory the

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